METHOD FOR DETERMINING A SHAPE SPACE FOR A SET OF MOLECULES USING MINIMAL METRIC DISTANCES

On page 1, at line 2, after the Title, and before "Field of the Invention", please insert:

B1 This application is a U.S. national phase application of International application PCT/US99/04343, filed February 26, 1999, and claims priority to U.S. provisional application serial no. 60/076,077, filed February 26, 1998.

Please replace the paragraph on page 12, beginning at line 27 with the following:

B2 Figs. 7A and 7B show flow charts illustrating a third aspect of the invention.

Please replace the paragraph on page 48, beginning at line 17, as follows:

B3 As illustrated in the flow chart of Figs. 7A and 7B, the closest structure is found by the following steps:

On page 74, replace the Abstract beginning at line 3 with the following.

NL: ABSTRACT NEEDS TO BE ON SEPERATE sheet

I describe several techniques for characterizing molecules based on the shapes of their fields. The minimal distance between two molecular fields is used as a shape-based metric, independent of the underlying chemical structure, and a high-dimensional shape space description of the molecules is generated. I then show how these attributes can be used in creating, characterizing, and searching databases of molecules based on field similarity. In particular, they allow searches of a database in sublinear time. Next, I extend the utility of this approach by describing a way to automatically break molecules into a series of fragments by using an ellipsoidal Gaussian decomposition. Not only can these fragments then be analyzed by the shape metric technique described above, but the parameters of the decomposition themselves can also be used to further organize and search databases. The most immediate application of these techniques is to pharmaceutical drug discovery and design.